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SHORT COMMUNICATION

The Lanczos method

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ABSTRACT

The Lanczos technique is one of the most frequently used numerical algorithms in matrix computations. We note that this procedure is one of the top 10 algorithms that exerted the greatest influence in the development and practice of science and engineering in the 20th century. Here we give an elementary exposition of this Lanczos method to solve the algebraic eigenvalue problem.

Keywords**:** Lanczos algorithm, Eigenvalue problem, Minimized iterations

1. INTRODUCTION

At the time of Lanczos research about the eigenvalue problem during World War II, most methods focused on finding the characteristic polynomial [1, 2] of matrices in order to find their eigenvalues. Lanczos original work [3] was also mostly concerned with this problem, however, he was trying to reduce the round-off errors in such calculations; he called his algorithm the ‘method of minimized iterations’ [4]. With the first implementations of the Lanczos procedure on the computers of the 1950’s, an undesirable numerical phenomenon was encountered: Due to the finite precision arithmetic, after certain number of steps the orthogonality among the Lanczos vectors was lost; this problem may be eliminated via additional labor to maintain the orthogonality. In exact arithmetic, the Lanczos technique can

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find only one proper vector associated to a multiple eigenvalue. The block method introduced by Golub-Underwood [5] works with multiple Lanczos vectors at a time and gives accurate calculation of multiple eigenvalues.

Calculating the inverse of a matrix [6, 7] proved to be a somewhat difficult task. To avoid matrix inversion, determined the matrix characteristic polynomial [1, 2, 8-12] was a preferred method; the roots of this polynomial provided the eigenvalues. Lanczos [3, 4] developed a progressive algorithm for the gradual construction of the minimal polynomial [1, 2, 13]. Starting from a trial vector and applying matrix transformations, Lanczos generated an iterated sequence of linearly independent vectors, each of them being a linear combination of the previous vectors; the procedure automatically comes to a halt when the proper degree of the polynomial has been reached. The coefficients of the final linear combination of the iterated vectors provide the coefficients of the minimal polynomial.

While Lanczos was working on his paper [3], A. M. Ostrowski [14] pointed out to Lanczos that his method paralleled the earlier research of Krylov [15]. Lanczos checked the relevant reviews in the reference journal Zentralblatt and informed Ostrowski that the literature available to him showed no evidence that the eigenvalue algorithm and the results he obtained have been found earlier. Using matrix transformation, Krylov created a sequence of consecutive vectors that had the smallest set of consecutive iterates that are linearly dependent. The coefficients of a vanishing combination are the coefficients of a divisor of the characteristic polynomial of the matrix; the space these vectors determine is called the Krylov subspace. Krylov´s iterative solver generated a huge class of approximate methods, among which the Lanczos algorithm [16] today is one of the most frequently used numerical methods in matrix computations [17].

Lanczos received credit for his discovery [18] because in 2000, the Editors of ‘Computing in Science and Engineering’, composed a list of 10 algorithms that exerted the greatest influence on the development and practice of science and engineering in the 20th century [19]; the Lanczos method was selected. Lanczos [3, 4] and Hestenes-Stiefel [20] initiate the implementation of Krylov subspace iteration techniques [6, 21].

2. LANCZOS METHOD: MINIMAL POLYNOMIAL, EIGENVALUES AND EIGENVECTORS

The Lanczos algorithm generates a set of orthogonal vectors which satisfy a recurrence relation; it connects three consecutive vectors with the result that each newly constructed vector is orthogonal to all of the previous ones. The numerical constants of the relation are determined during the process from the condition that the length of each newly produced vector should be minimal. After a certain number of iterations (minimized iterations) in view of the Cayley-Hamilton-Frobenius identity [1, 2, 22], the last vector must become a linear combination of the previous vectors. The method, though indisputably an elegant one, had a serious limitation; in case of eigenvalues with considerable dispersion, the successive iterations will increase the gap, the large proper values will monopolize the scene, and because of rounding errors the small eigenvalues begin to lose value. After a few iterations they will be practically drowned out; a certain kind of eigenvalue identity had to be established. Lanczos developed a modification of the method that protected the small proper values by balancing the distribution of amplitudes in the most equitable fashion; to achieve this, the coefficients of the linear combination of the iterated vectors are determined in such way that the amplitude of the new vector should be minimal. The generated vectors were orthogonal to each other (successive orthogonalization).

Lanczos first considered symmetric matrices, $A = A^T$, and set out to find the minimal polynomial for the eigenvalue problem $A\vec{u} = \lambda\vec{u}$, and he generates a sequence of trial vectors, resulting in a successive set of polynomials [23]. The process starts with $\vec{b}_0$ randomly selected, then we construct the next vector in according with the rule:

$$\vec{b}_1 = A\vec{b}_0 - \alpha_0 \vec{b}_0 , \tag{1}$$

where: the value of α_0 must imply that $\vec{b}_1^2$ is a minimum, thus:

$$\vec{b}_0^2 \alpha_0 = \vec{b}_0 \cdot A\vec{b}_0 , \qquad \vec{b}_1 \cdot \vec{b}_0 = 0. \tag{2}$$

Similarly:

$$\vec{b}_2 = A\vec{b}_1 - \alpha_1 \vec{b}_1 - \beta_0 \vec{b}_0 , \tag{3}$$

with the parameters α_1 and β_0 such that $\vec{b}_2^2$ has a minimum value, therefore:

$$\vec{b}_1^2 \alpha_1 = \vec{b}_1 \cdot A\vec{b}_1 , \quad \vec{b}_0^2 \beta_0 = \vec{b}_0 \cdot A\vec{b}_1 = \vec{b}_1^2 , \quad \vec{b}_2 \cdot \vec{b}_0 = \vec{b}_2 \cdot \vec{b}_1 = 0, \tag{4}$$

and:

$$\vec{b}_3 = A\vec{b}_2 - \alpha_2\vec{b}_2 - \beta_1\vec{b}_1 , \quad \vec{b}_2^2 \alpha_2 = \vec{b}_2 \cdot A\vec{b}_2 , \quad \vec{b}_1^2 \beta_1 = \vec{b}_1 \cdot A\vec{b}_1 = \vec{b}_2^2 , \quad \vec{b}_3 \cdot \vec{b}_r = 0, \quad r = 0,1,2, \tag{5}$$

for a minimum value of $\vec{b}_3^2$, etc. Then, the algorithm established by Lanczos is now:

$\vec{b}_0$ randomly selected vector,

$$A = A^T, \quad \vec{b}_1 = (A - \alpha_o I)\,\vec{b}_0, \quad \vec{b}_2 = (A - \alpha_1 I)\,\vec{b}_1 - \beta_0 \vec{b}_0 , \ \cdots$$
$$\cdots \ \vec{b}_m = (A - \alpha_{m-1} I)\,\vec{b}_{m-1} - \beta_{m-2} \vec{b}_{m-2} = \vec{0} , \quad \text{[end of the process]}, \tag{6}$$

with the famous three-member recurrence [16], such that:

$$\vec{b}_r^2 \alpha_r = \vec{b}_r \cdot A\vec{b}_r , \ \ r = 0, 1, \dots, m-1,$$
$$\vec{b}_j^2 \beta_j = \vec{b}_j \cdot A\vec{b}_{j+1} = \vec{b}_{j+1}^2 , \ \ j = 0, 1, \dots, m-2,$$
$$\vec{b}_a \cdot \vec{b}_c = 0, \quad a = 1, 2, \dots, m-1 ; \quad c = 0, 1, \dots, a-1. \tag{7}$$

At every step of the Lanczos method a new $\vec{b}_{j+1}$ vector is found by projecting the $A\vec{b}_j$ vector into the subspace spanned by the previous Lanczos vectors and choosing $\vec{b}_{j+1}$ to be the component of $A\vec{b}_j$ orthogonal to the projection. In Lanczos view we reached the order of the minimal polynomial [13, 24-26] $m \leq n$ for $A_{nxn} = A^T$. Unfortunately, in finite precision arithmetic, the process may reach a state where β_k is very small for $k < m$ before the full order of the minimal polynomial is obtained. This phenomenon, at the time not fully understood, contributed to the method's bad numerical reputation in the 1960's.

This algorithm generates a sequence of polynomials [23] to construct the minimal polynomial of a symmetric matrix:

$$p_0(\lambda) = 1,\ p_1(\lambda) = \lambda - \alpha_0\ ,\ \ p_r(\lambda) = (\lambda - \alpha_{r-1})\, p_{r-1}(\lambda) - \beta_{r-2}\, p_{r-2}(\lambda),\ \ r = 2, 3, \ldots\ , \quad (8)$$

thus the corresponding minimal polynomial is given by:

$$p_m(\lambda) = (\lambda - \alpha_{m-1})\, p_{m-1}(\lambda) - \beta_{m-2}\, p_{m-2}(\lambda), \quad (9)$$

where m was determined in the process (6) [$\vec{b}_m = \vec{0}$]. From (8), the Lanczos polynomials can be expressed as determinants of matrices generated by the parameters (7), in fact [27]:

$$p_r(\lambda) = \det(\lambda\, I_{rxr} - L_{rxr})\ , \quad r = 1, 2, 3, \ldots\ ; \quad L = \begin{pmatrix} \alpha_0 & \beta_0 & 0 & \cdots & 0 \\ 1 & \alpha_1 & \beta_1 & \cdots & \\ 0 & 1 & \alpha_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ 0 & 0 & 0 & 1 & \alpha_{r-1} \end{pmatrix}, \quad (10)$$

that is:

$$L_{1X1} = (\alpha_0), \quad L_{2X2} = \begin{pmatrix} \alpha_0 & \beta_0 \\ 1 & \alpha_1 \end{pmatrix}, \quad L_{3x3} = \begin{pmatrix} \alpha_0 & \beta_0 & 0 \\ 1 & \alpha_1 & \beta_1 \\ 0 & 1 & \alpha_2 \end{pmatrix}, \quad L_{4x4} = \begin{pmatrix} \alpha_0 & \beta_0 & 0 & 0 \\ 1 & \alpha_1 & \beta_1 & 0 \\ 0 & 1 & \alpha_2 & \beta_2 \\ 0 & 0 & 1 & \alpha_3 \end{pmatrix},$$

etc.

For nonsymmetric matrices, the transpose of A participates in the implementation of the Lanczos technique, thus $\vec{b}_0$ and $\vec{t}_0$ are randomly selected vectors to construct:

$$\vec{b}_1 = A\vec{b}_0 - \alpha_0\, \vec{b}_0\ , \quad \vec{t}_1 = A^T\vec{t}_0 - \alpha_0\, \vec{t}_0\ , \quad \vec{b}_0 \cdot \vec{t}_1 = \vec{t}_0 \cdot \vec{b}_1 = 0, \quad (\vec{b}_0 \cdot \vec{t}_0)\alpha_0 = \vec{t}_0 \cdot A\vec{b}_0 = \vec{b}_0 \cdot A^T\vec{t}_o.$$

Similarly:

$$\vec{b}_2 = A\vec{b}_1 - \alpha_1\, \vec{b}_1 - \beta_0\, \vec{b}_0\ , \quad \vec{t}_2 = A^T\vec{t}_1 - \alpha_1\, \vec{t}_1 - \beta_0\, \vec{t}_0\ , \quad \vec{b}_2 \cdot \vec{t}_r = \vec{t}_2 \cdot \vec{b}_r = 0, \quad r = 0, 1,$$

$$(\vec{b}_1 \cdot \vec{t}_1)\, \alpha_1 = \vec{t}_1 \cdot A\vec{b}_1 = \vec{b}_1 \cdot A^T\vec{t}_1\ , \quad (\vec{b}_0 \cdot \vec{t}_0)\, \beta_0 = \vec{t}_1 \cdot A\vec{b}_0 = \vec{b}_0 \cdot A^T\vec{t}_1 = \vec{b}_1 \cdot \vec{t}_1\ ;$$

in general, for $k = 0, 1, 2, \ldots$:

$$\vec{b}_{k+2} = A\vec{b}_{k+1} - \alpha_{k+1}\,\vec{b}_{k+1} - \beta_k\,\vec{b}_k\,, \qquad \vec{t}_{k+2} = A^T\vec{t}_{k+1} - \alpha_{k+1}\,\vec{t}_{k+1} - \beta_k\,\vec{t}_k\,,$$

$$\left(\vec{b}_k \cdot \vec{t}_k\right)\alpha_k = \vec{t}_k \cdot A\vec{b}_k = \vec{b}_k \cdot A^T\vec{t}_k\,,\ \left(\vec{b}_k \cdot \vec{t}_k\right)\beta_k = \vec{t}_{k+1} \cdot A\vec{b}_k = \vec{b}_k \cdot A^T\vec{t}_{k+1} = \vec{b}_{k+1} \cdot \vec{t}_{k+1}\,, \tag{11}$$

$\vec{b}_a \cdot \vec{t}_c = \vec{t}_a \cdot \vec{b}_c = 0, \quad a = 1, 2, \ldots, m-1\ ; \quad c = 0, 1, \ldots, a-1$ [biorthogonality];

this process stops when $\vec{b}_m = \vec{t}_m = \vec{0}$, $m \le n$, and the minimal polynomial of A is given by (8) and (9) with the parameters α_k and β_k determined in (11). If $A = A^T$, then the expressions (11) imply (7) because $\vec{b}_k = \vec{t}_k$. Due to the finite precision arithmetic, after some number of steps the biorthogonality of the Lanczos vectors is lost, it is necessary additional work to maintain the orthogonality during the process.

The characteristic polynomial [1, 2, 8-12, 28-30] permits to obtain the eigenvalues of a matrix. The quantities $p_j(\lambda_k)$ and $\vec{b}_r \cdot \vec{t}_r$ are important to determine the corresponding eigenvectors. In fact, we consider an arbitrary matrix A_{nxn} , its eigenvalue problem is complete it its transpose participates in the algorithm:

$$A\vec{u}_r = \lambda_r\,\vec{u}_r, \qquad A^T\vec{v}_r = \lambda_r\,\vec{v}_r\,, \tag{12}$$

because both matrices have the same characteristic polynomial. If we accept the notation:

$$Q_j = \vec{b}_j \cdot \vec{t}_j \ne 0, \qquad j = 0, 1, \ldots, m-1, \tag{13}$$

then the Lanczos method gives expressions to construct linearly independent proper vectors:

$$\begin{gathered} \vec{u}_k = \frac{1}{Q_0}\,\vec{b}_0 + \frac{p_1(\lambda_k)}{Q_1}\,\vec{b}_1 + \frac{p_2(\lambda_k)}{Q_2}\,\vec{b}_2 + \cdots + \frac{p_{m-1}(\lambda_k)}{Q_{m-1}}\,\vec{b}_{m-1}\,, \\ k = 1, \ldots, N, \\ \vec{v}_k = \frac{1}{Q_0}\,\vec{t}_0 + \frac{p_1(\lambda_k)}{Q_1}\,\vec{t}_1 + \frac{p_2(\lambda_k)}{Q_2}\,\vec{t}_2 + \cdots + \frac{p_{m-1}(\lambda_k)}{Q_{m-1}}\,\vec{t}_{m-1}\,, \end{gathered} \tag{14}$$

where: N is the number of different eigenvalues. If some λ_r is multiple, then we may apply the Lanczos procedure for several $\vec{b}_0$ and $\vec{t}_0$ and thus to obtain all independent eigenvectors associated to these multiple proper value. Let's remember that there are $M_j + 1 - m_j$ independent proper vectors associated with each different λ_j, where M_j is the multiplicity of this eigenvalue and m_j indicates the presence of the factor $(\lambda - \lambda_j)^{m_j}$ into the minimal polynomial; when $N = n$, hence also $m = n$, the relations (14) give independent vectors with the known property [1] $\vec{u}_j \cdot \vec{v}_k = 0,\ j \ne k$, that is:

$$\sum_{r=0}^{n-1} \frac{1}{Q_r}\, p_r(\lambda_q)\, p_r(\lambda_c) = 0, \qquad q \neq c. \tag{15}$$

This Lanczos-Hestenes-Stiefel method was originally developed as a direct algorithm to solve a nxn linear system, and it is useful when employed [31] as an iterative approximation technique for solving large sparse systems with nonzero entries occurring in predictable patterns. These problems frequently arise in the solution of boundary value problems; good results are obtained in only about $\sqrt{n}$ iterations; employed in this way, the method is preferred over Gaussian elimination.

The iterative Leverrier-Faddeev-Sominsky-Souriau-Frame procedure [6, 8, 12, 29, 32-43] permits to determine the inverse matrix A^{-1}, however, Lanczos algorithm gives us an alternative way for the inversion of a matrix. In fact, we accept that rank $A = n$ [44] to construct the nxn matrices:

$$B = \left(\frac{\vec{b}_0}{Q_0}\ \frac{\vec{b}_1}{Q_1}\ \cdots\ \frac{\vec{b}_{n-1}}{Q_{n-1}}\right), \qquad T = \left(\vec{t}_0\ \vec{t}_1 \cdots \vec{t}_{n-1}\right), \qquad B^T\, T = I, \tag{16}$$

then:

$$R \equiv T^T A B = \begin{pmatrix} \alpha_0 & 1 & 0 & 0 & \cdots & 0 \\ \beta_0 & \alpha_1 & 1 & 0 & \cdots & 0 \\ 0 & \beta_1 & \alpha_2 & \ddots & \ddots & 0 \\ 0 & 0 & \beta_2 & \ddots & 1 & \vdots \\ \vdots & \vdots & \vdots & \ddots & \alpha_{n-2} & 1 \\ 0 & 0 & 0 & \cdots & \beta_{n-2} & \alpha_{n-1} \end{pmatrix}. \tag{17}$$

In general, it is more easy to obtain [45, 46] the inverse of the tridiagonal matrix R than A^{-1}, thus when $\det R = \det A \neq 0$, then (17) implies the Lanczos expression:

$$A^{-1} = B\, R^{-1}\, T^T. \tag{18}$$

Hence the Lanczos vectors provide a similarity transformation [2] under which A acquires a tridiagonal structure.

3. CONCLUSIONS

The Lanczos process [46-49] solves the standard eigenvalue problem (12) for square matrices, then it must be interesting to realize its implementation for the rectangular case known as 'shifted eigenvalue problem' [50-53]. We emphasize that this algorithm can be applied to several random vectors $\vec{b}_0$ and $\vec{t}_0$ to determine all independent eigenvectors associated to a multiple proper value. The Lanczos method gives the minimal polynomial for the matrix under analysis, which is important in the Gower's procedure [36] to construct proper vectors via the Leverrier-Faddeev's technique [6, 8, 12, 29, 32-43].

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